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## Supporting Information

### Structural insights of Ketanserin salts with aliphatic acids and their physiochemical properties

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Parameters 2.367	KTS.SA.H2O	KTS.SA.2H2O	KTS.MA	KTS.FA
Formula	C <sub>22</sub> H <sub>23</sub> FN <sub>3</sub> O <sub>3</sub> :H <sub>3</sub>	C <sub>22</sub> H <sub>23</sub> FN <sub>3</sub> O <sub>3</sub> :	C <sub>22</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>3</sub> :	C <sub>22</sub> H <sub>23</sub> FN <sub>3</sub> O <sub>3</sub> :
	N <sub>3</sub> S:H <sub>2</sub> O	H <sub>2</sub> NO <sub>3</sub> S:2(H <sub>2</sub> O)	C <sub>4</sub> H <sub>3</sub> O <sub>4</sub>	C <sub>4</sub> H <sub>3</sub> O <sub>4</sub>
<i>M<sub>r</sub></i>	511.54	528.55	510.49	511.50
crystal shape	Needle	block	Block	Block
crystal colour	Colourless	colourless	Colourless	Colourless
crystal system	Triclinic	Triclinic	Monoclinic	Monoclinic
space group	<i>P</i> <sup>-1</sup>	<i>P</i> <sup>-1</sup>	<i>P</i> 2 <sub>1</sub> / <i>n</i>	<i>P</i> 2 <sub>1</sub> / <i>c</i>
<i>T</i> , K	100	301.00	298(2)	298(2)
λ(Mo-K <sub>α</sub> )/Å	0.71073	0.71073	0.71073	0.71073
<i>a</i> /Å	8.554(3)	9.104(3)	6.018(5)	6.662(2)
<i>b</i> /Å	10.936(5)	10.937(4)	31.707(2)	21.965(1)
<i>c</i> /Å	12.526(5)	12.774(5)	12.500(1)	16.468(1)
<i>α</i> <sup>0</sup>	85.91(2)	86.214(11)	90	90
<i>β</i> <sup>0</sup>	76.418(19)	71.917(10)	96.98(2)	91.69(1)
<i>γ</i> <sup>0</sup>	87.737(17)	82.894(12)	90	90
<i>V</i> /Å <sup>3</sup>	1135.8(8)	1199.3(7)	2368.0(3)	2408.7(4)
<i>Z</i>	2	2	4	4
<i>D<sub>c</sub></i> / g cm <sup>-3</sup>	1.496	1.464	1.432	1.411
<i>μ</i> , mm <sup>-1</sup>	0.204	0.199	0.110	0.108
2θ range [°]	2.43-27.48	2.36-25	2.53-26.40	2.64-27.48
limiting indices	-11 ≤ <i>h</i> ≤ 11	-10 ≤ <i>h</i> ≤ 10	-7 ≤ <i>h</i> ≤ 7	-8 ≤ <i>h</i> ≤ 8
	-14 ≤ <i>k</i> ≤ 14	-12 ≤ <i>k</i> ≤ 12	-39 ≤ <i>k</i> ≤ 39	-28 ≤ <i>k</i> ≤ 28
	-16 ≤ <i>l</i> ≤ 16	-15 ≤ <i>l</i> ≤ 15	-15 ≤ <i>l</i> ≤ 15	-21 ≤ <i>l</i> ≤ 21
<i>F</i> (000)	538	556	1068	1072
total reflections	43374	18053	40219	49293
unique reflections	5194	4199	4869	5537
reflection at <i>I</i> >	4102	2183	2961	3809
2σ ( <i>I</i> )				
No. of parameters	333	356	343	339
<i>R</i> <sub>1</sub> , <i>I</i> > 2σ ( <i>I</i> )	0.045	0.090	0.047	0.053
<i>wR</i> <sub>2</sub> <i>I</i> > 2σ ( <i>I</i> )	0.109	0.264	0.148	0.115
GoF on <i>F</i> <sup>2</sup>	1.051	1.061	1.123	1.062
CCDC Nos	2372349	2372347	2372346	2372345

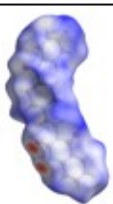
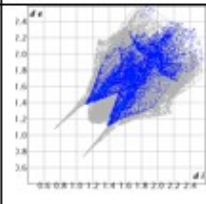
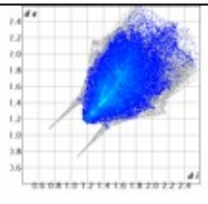
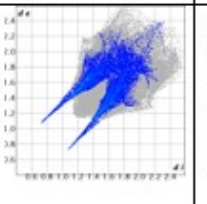
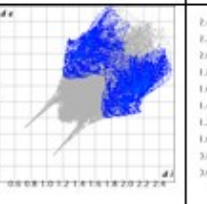
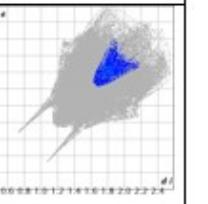
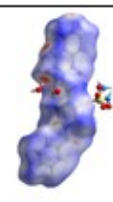
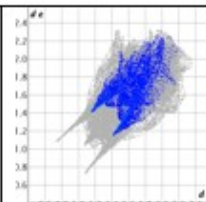
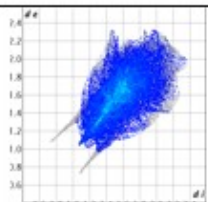
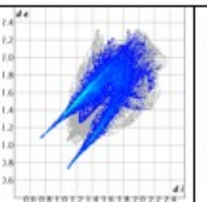
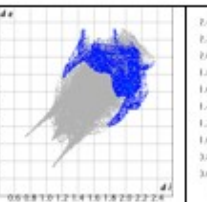
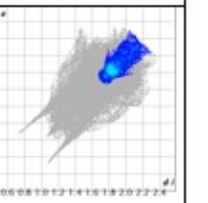
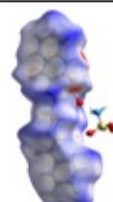
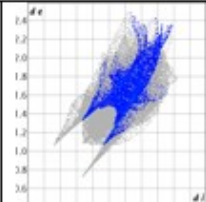
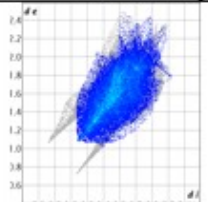
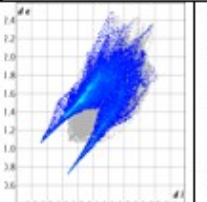
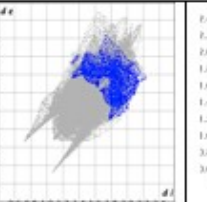
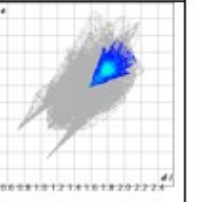

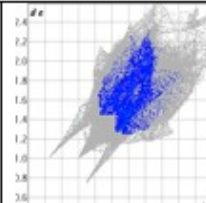
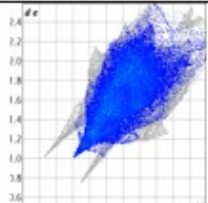
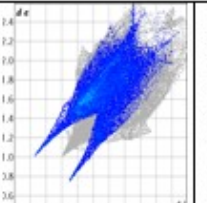
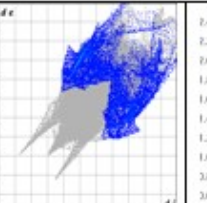
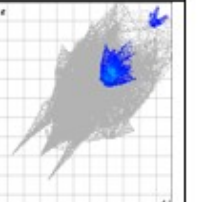
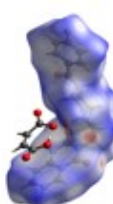
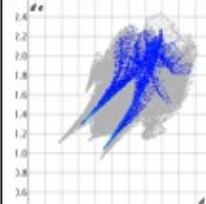
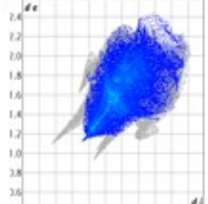
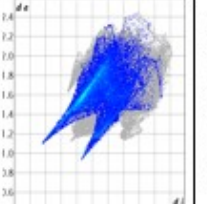
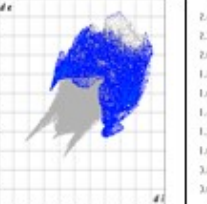
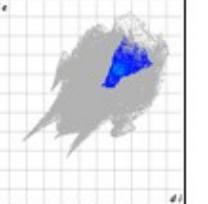
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**Table S1.** Crystallographic lattice parameters of KTS salts

Solid forms	<i>D</i> –H··· <i>A</i>	<i>D</i> –H(Å)	H··· <i>A</i> (Å)	<i>D</i> – <i>A</i> (Å)	<i>D</i> –H··· <i>A</i> (°)
<b>KTS.SA (DH)</b>	N2–H2···O3	0.86	1.98	2.823(5)	164.7
	N3–H3···O5	0.98	1.93	2.827(5)	151.7
	O8–H8a···O4 <sup>2</sup>	0.91	1.89	2.778(1)	166.7
	O8–H8b···O2	0.94	1.87	2.799(6)	166.8
	O10–H10c···O8	0.85	2.08	2.732(1)	133.6
	O10–H10d···O6 <sup>3</sup>	0.85	1.54	2.39(2)	179.6
<b>KTS.SA (MH)</b>	N2–H2···O31	0.90(3)	1.92(3)	2.793(2)	165(2)
	O7–H7A···O2	0.86(4)	1.96(4)	2.808(2)	168(3)
	O7–H7B···O62	0.84(3)	2.04(3)	2.873(3)	171(3)
	N3–H3···O43	0.91(3)	1.95(3)	2.846(2)	166(2)
<b>KTS.MA</b>	N3–H3···O6	0.94(3)	1.93(3)	2.774(2)	149(2)
	O4–H4A···O6	0.82	1.61	2.426(3)	177.9
<b>KTS.FA</b>	O5–H5···O6	0.82	1.77	2.563(2)	162.5
	N1–H1···O11	0.92(3)	1.70	2.798(2)	155(2)
	N3–H3···O7	0.98	1.93(3)	2.681(2)	174.4

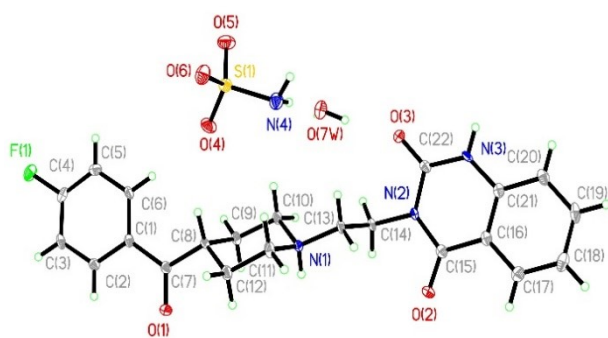
**Table S2:** Hydrogen bond geometry (Å/°) of molecular adducts of KTS.

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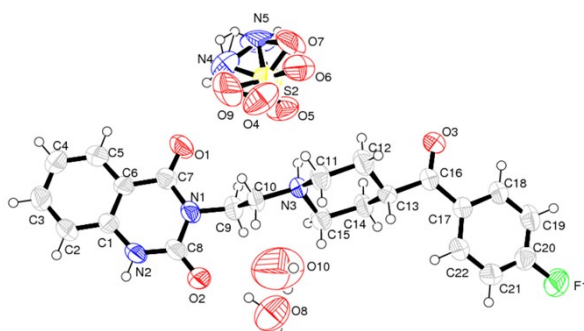
	F-H	H-H	H-O	H-C	C-C
					
KTS	9.6%	45.2%	17%	17.6%	3%
Total contact population = 92.4%					
					
KTS-SA-DH	7.4%	39.6%	29.9%	7.1%	9.3%
Total contact population = 93.3%					
					
KTS-SA-MH	8.2%	40.6%	29.6%	5.6%	10.8%
Total contact population = 94.8%					
					
KTS-FA	7.3%	37.9%	26.7%	14.2%	4.7%
Total contact population = 90.8%					
					
KTS-MA	8%	37%	27.7%	15.3%	3.8%
Total contact population = 91.8%					

**Table S3:** Hirshfeld Analysis of KTS and its salts

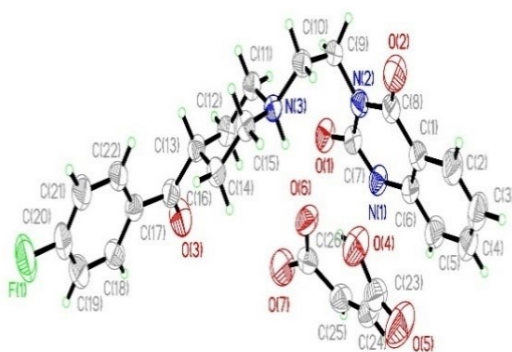
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(a)

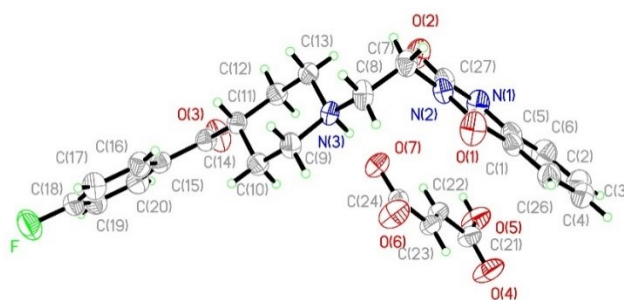


(b)



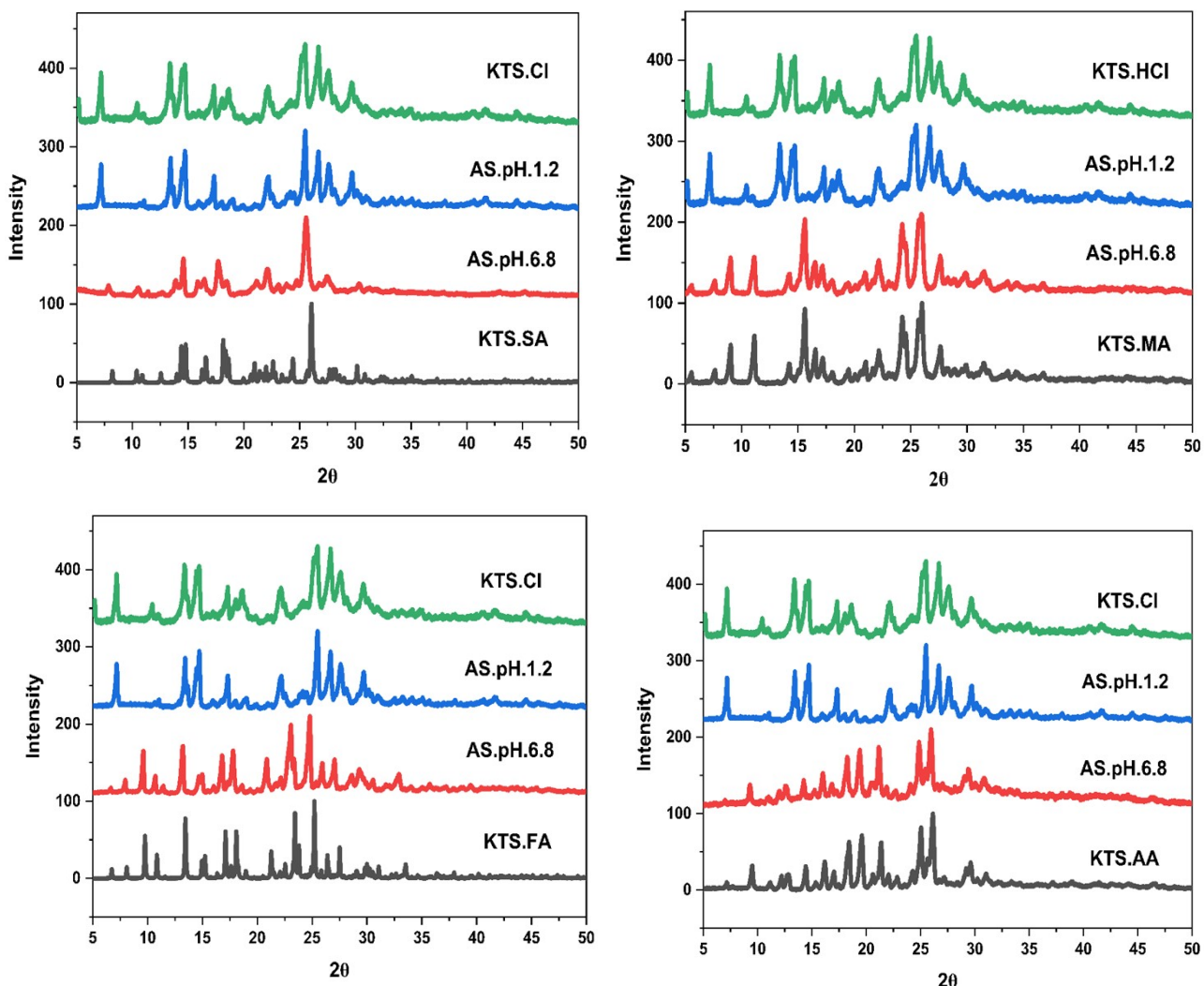
(c)

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(d)

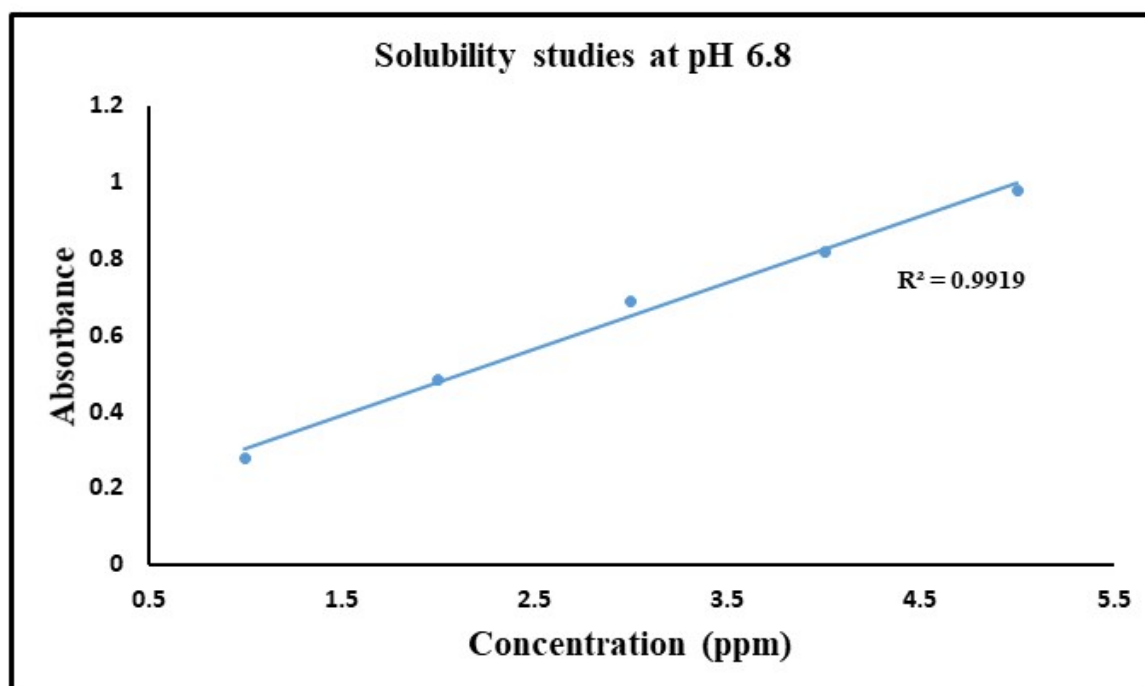
**Figure S1:** ORTEP view of (a) KTS.SAMH, (b) KTS.SA.DH, (c) KTS.MA (d) KTS.FA salts. Herein, the thermal ellipsoids are drawn with a 50% probability.



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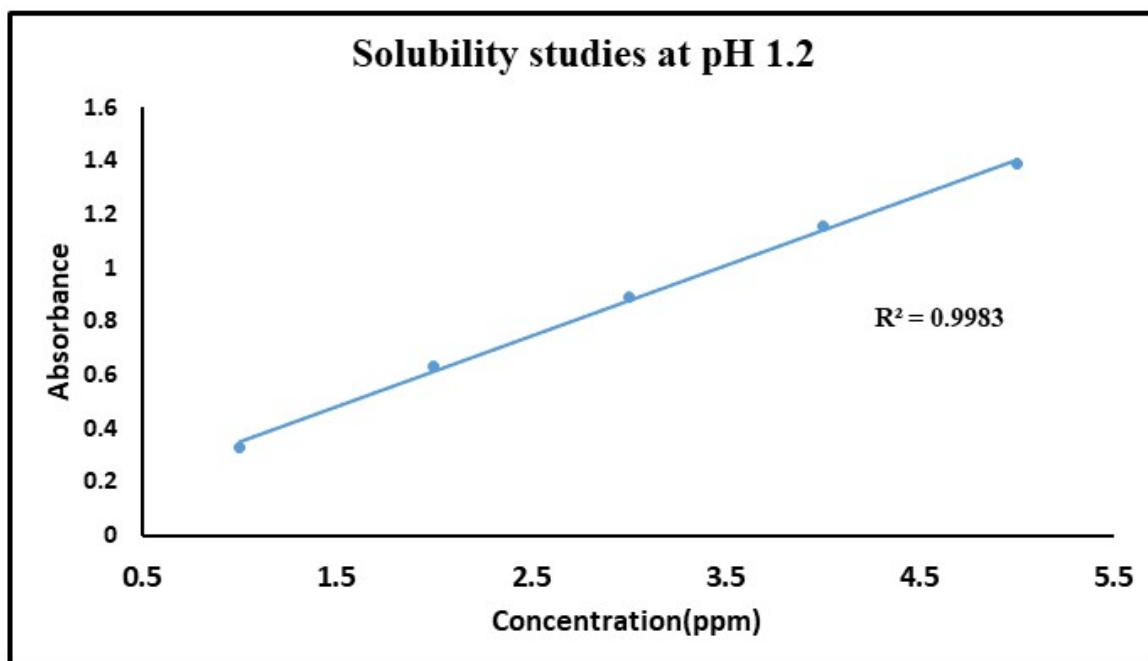
**Figure S2.** PXRD Analysis of all molecular adducts after solubility in both pH 1.2 and 6.8 media

**Solubility studies of KTS and its salts in both pH 1.2 and 6.8 medium:**





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#### Standard Table for KTS in pH 6.8

ppm	Absorbance
1	0.278
2	0.482
3	0.688
4	0.82
5	0.978

#### Unknown Table of KTS in pH 6.8 after applying dilution factor

S.No	Sample Name	Absorbance			Concentration (ppm)			Standard Deviation	Average Concentration (ppm)	After adding the dilution factor (mg/mL)
1	KTS.AA	0.529	0.532	0.534	2.3140	2.3311	2.3425	0.0144	2.3292	2.33
2	KTS.FA	0.74	0.743	0.739	3.5182	3.5353	3.5125	0.0119	3.5220	3.52
3	KTS.MA	0.565	0.563	0.566	2.5195	2.5080	2.5252	0.0087	2.5176	2.52
4	KTS.SA	0.958	0.962	0.959	4.7624	4.7852	4.7681	0.0119	4.7719	15.41
5	KTS.TA	1.027	1.024	1.019	5.1561	5.1390	5.1105	0.0231	5.1352	3.59
6	KTS.HCl	0.862	0.868	0.865	4.2145	4.2487	4.2316	0.0171	4.2316	4.23
7	KTS	0.372	0.379	0.375	1.4180	1.4579	1.4351	0.0200	1.4370	1.44



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**Standard Table for KTS in pH 1.2**

ppm	Absorbance
1	0.332
2	0.633
3	0.891
4	1.156
5	1.392

**Unknown Table of KTS in pH 1.2 after applying dilution factor**

S.No	Sample Name	Absorbance			Concentration (ppm)			Standard Deviation	Average Concentration (ppm)	After adding the dilution factor (mg/mL)
1	KTS.AA	0.699	0.701	0.696	2.3133	2.3209	2.3020	0.0095	2.3121	2.31
2	KTS.FA	0.723	0.719	0.716	2.4040	2.3889	2.3775	0.0132	2.3901	2.39
3	KTS.MA	0.899	0.901	0.907	3.0687	3.0763	3.0990	0.0157	3.0813	3.08
4	KTS.SA	0.652	0.659	0.66	2.1358	2.1622	2.1660	0.0165	2.1547	2.14
5	KTS.TA	0.653	0.661	0.649	2.1396	2.1698	2.1245	0.0231	2.1446	3.59
6	KTS.HCl	0.601	0.593	0.592	1.9432	1.9130	1.9092	0.0186	1.9218	1.92
7	KTS	0.442	0.456	0.438	1.3426	1.3955	1.3275	0.0357	1.3552	1.36